HOW to EVALUATE COMPOUNDS

1. Generate library of possible compounds on the computer

ISIS, UNITY

2. Build 3D model of each compound in the library

CONCORD

3. Use conformational flexible searching to determine which of the compounds are able to match the pharmacophore model

ISIS, UNITY, DGEOM

4. Generate "family" of low-energy conformations for each remaining molecule

WIZARD, DGEOM

5. For each molecule, determine whether any of the low-energy conformations match the pharmacophore

DISCO, APEX, Catalyst

6. Dock the remaining conformations

DOCK

7. Flexibly dock the good ones

AUTO DOCK

8. Score them (evaluate the strain energy) using various methods

CHARMM, MMFF

9. Synthesize the best candidates